

Receiver operation characteristics of quantum state discrimination

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Abstract. We provide a description of the problem of the discrimination of two quantum states in terms of receiver operation characteristics analysis, a prevalent approach in classical statistics. Receiver operation characteristics diagrams provide an expressive representation of the problem, in which quantities such as the fidelity and the trace distance also appear explicitly. In addition we introduce an alternative quantum generalization of the classical Bhattacharyya coefficient. We evaluate our quantum Bhattacharyya coefficient for certain situations and describe some of its properties. These properties make it applicable as another possible quantifier of the similarity of quantum states.

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1. Introduction

The problem of discriminating two quantum states is a central, well-understood problem of quantum information processing: given a quantum system along with the prior information that it is in either of two possible given states with some probability, we have to tell, as accurately as possible, in which of its possible states the system is. There has been a tremendous and successful effort, resulting in a detailed understanding of many facets of the problem. Instead of recapitulating these results here, we refer to the excellent reviews in Refs. [1, 2].

Note that the discrimination problem has its antecedents in classical statistics. Given a sample drawn from either of two possible random variables with the same

possible set of values but different distribution, a typical task of statistics is to decide which of the variables were actually used to draw the sample. This relates to the idea of receiver operation characteristics (ROC) analysis, which can be simply understood from one of its typical applications. The task is to decide whether a patient suffers from a given illness. In order to do so, a test is carried out, from which a conclusion is drawn. Of course, there may be four cases. If we conclude that the patient is ill, this maybe a true or a false positive depending on whether we succeed or fail. True and false negatives can be understood similarly for the negative conclusion. The rate of these events depend of course on the test we carry out and the rules to draw the conclusion. A given definition of the test and the processing rules specify a *discriminator*. The idea of ROC analysis is to draw the true positive rate as a function of the false positive rate for a given discriminator. Visualizing all the possible discriminators in such a way leads to a couple very intuitive and useful techniques termed as ROC analysis (see Ref. [3] for a review).

The analogy with quantum state discrimination is clear: if we consider one of the possible quantum states to be the “positive”, the other one to be the “negative” state of the system, we have to decide if in reality it is in the “positive” state. Though in our case there is no natural assymetry in the choice of the “positive” or “negative” state, the technique is, as we shall see, applicable in this case, too. The classical limit of this quantum scenario is the case of the discrimination of two probability distributions, as described above.

Throughout this paper we elaborate on the application of ROC analysis to the quantum scenario. In order to do so, in Section 2 we describe the case of the discrimination of classical random variables, in terms of ROC curves. Here we derive those facts of ROC analysis which we shall use in the rest of the paper. It is of special interest here to understand the classical Bhattacharyya-coefficient [4], a quantity characterizing the similarity of two probability distribution, as a certain integral of the ROC curve. Though most of these are available in the literature of ROC analysis, it is useful to describe them in detail for sake of self-consistency. In Section 3 we describe the case of ambiguous discrimination of two quantum states. We provide a full analysis of the case of two pure states and that of two mixed states with common support, and describe the most general case of two arbitrary states, too. We find the representation of trace distance and fidelity in the ROC curve. In addition, we introduce and analyze a version of quantum Bhattacharyya coefficient as an integral of a ROC curve, just like in the classical case. This approach is different from the quantum Bhattacharyya coefficient that was introduced in the literature (see e.g. Ref. [5]). We explore several properties of this quantity which make it a useful similarity measure [6]. In Section 4 we outline the case of unambiguous state discrimination in the ROC picture. In Section 5 our results are summarized and conclusions are drawn.

2. Classical ROC curves

Let us consider the problem of discriminating two classical random variables with the same finite range (that is, the discrimination of two probability distributions). Though in ROC analysis it is common to consider empirical rates, the technique works also for probability distributions and conditional probabilities, too, and this is the way we follow. First we consider the case of two binary variables.

2.1. Two binary variables

Assume that we have a binary random variable (i.e. a classical bit) with 0 and 1 as possible values. The variable can be distributed according to two possible distributions

$$(p, 1 - p) \quad \text{or} \quad (q, 1 - q), \quad (1)$$

where $p, q \in [0, 1]$. We know these distributions in advance. We want to decide whether the variable is distributed according to the first of these. We denote this event by \mathfrak{P} (“positive”), while the complementary event with \mathfrak{N} (“negative”). Let $\Pr(\mathfrak{P}) = \lambda \in [0, 1]$ be also given in advance. We measure the variable, the measurement yields the actual value. We denote the two possible events with the respective values 0 and 1. The task is to guess which one is the true distribution. We denote the events corresponding to our two possible guesses by \mathfrak{p} and \mathfrak{n} .

By choosing a particular classifier we fix the way how we deduce the guess $\mathfrak{p}/\mathfrak{n}$ from the result of the observation 0/1. The properties of the possible classifiers will be studied in the ROC space: a classifier is represented here by a point, on the vertical axis we have the conditional probability $\Pr(\mathfrak{p}|\mathfrak{P})$, while on the horizontal axis we measure $\Pr(\mathfrak{p}|\mathfrak{N})$. If we were to repeat the procedure on a large number samples all prepared in the same way, the first quantity describes the *true positive rate*, while the second one the *false positive rate*.

For a classifier we consider a general random mapping characterized by the following conditional probabilities:

$$\begin{aligned} \Pr(\mathfrak{p}|0) &= p_{a,p}, \\ \Pr(\mathfrak{n}|1) &= p_{a,n}, \\ \Pr(\mathfrak{n}|0) &= 1 - p_{a,p}, \\ \Pr(\mathfrak{p}|1) &= 1 - p_{a,n}, \end{aligned} \quad (2)$$

with the *acceptance probabilities* $p_{a,p}, p_{a,n} \in [0, 1]$. Setting $p_{a,p} = p_{a,n} = 1$ corresponds to the deterministic case when we consider 0 as the indicator of \mathfrak{P} and 1 that of \mathfrak{N} . Alternatively, we may allow for some randomness in our choice. Note that the choice of the distribution ($\mathfrak{P}/\mathfrak{N}$), the measurement result (0/1) and the conclusion ($\mathfrak{p}/\mathfrak{n}$), as random variables, form a Markov-chain.

In the given situation we have

$$\Pr(\mathfrak{p}|\mathfrak{P}) = \Pr(\mathfrak{p}|0, \mathfrak{P}) \Pr(0|\mathfrak{P}) + \Pr(\mathfrak{p}|1, \mathfrak{P}) \Pr(1|\mathfrak{P}). \quad (3)$$

We have $\Pr(\mathbf{p}|0, \mathfrak{P}) = \Pr(\mathbf{p}|0)$ and $\Pr(\mathbf{p}|1, \mathfrak{P}) = \Pr(\mathbf{p}|1)$ from the Markov chain, and these probabilities are known from Eq. (2), while the rest of the probabilities is known from (1), so we have

$$\Pr(\mathbf{p}|\mathfrak{P}) = p_{a,p}p + (1 - p_{a,n})(1 - p). \quad (4)$$

For the false positive rate we have

$$\Pr(\mathbf{p}|\mathfrak{N}) = \Pr(\mathbf{p}|0, \mathfrak{N}) \Pr(0|\mathfrak{N}) + \Pr(\mathbf{p}|1, \mathfrak{N}) \Pr(1|\mathfrak{N}), \quad (5)$$

which evaluates along the same lines of thought as

$$\Pr(\mathbf{p}|\mathfrak{N}) = p_{a,p}q + (1 - p_{a,n})(1 - q). \quad (6)$$

Thus for a given p and q we have to plot $p_{a,p}p + (1 - p_{a,n})(1 - p)$ against $p_{a,p}q + (1 - p_{a,n})(1 - q)$ for all possible $(p_{a,p}, p_{a,n})$ pairs as parameters to obtain the ROC diagram for all the possible classifiers. Note that it does not depend on λ : it characterizes the classifier based on the two probability distributions to be distinguished, and not the prior probability of having one of them at hand.

To visualize the behavior of the point set in the ROC space defined by Eqs. (6) and (4), we express $(1 - p_{a,n})$ from Eq. 6:

$$0 \leq (1 - p_{a,n}) = \frac{x - p_{a,p}q}{1 - q} \leq 1, \quad (7)$$

where we have indicated the bounds on $(1 - p_{a,n})$. Substituting this to (4), after some algebra we have

$$y = \frac{1 - p}{1 - q}x + \left(p - \frac{1 - p}{1 - q}q\right)p_{a,p} = Ax + Bp_{a,p}. \quad (8)$$

(We exclude the trivial cases when $p, q = 0$ or 1 .) For $p_{a,p} = 0$ this defines a line through the origin of the ROC space. For $p_{a,p} = 1$ we get a parallel line, above or below the other one, depending on the sign of B . The available region is within these parallel lines. However, $p_{a,p}$ may have stronger bounds due to the bounds in Eq. (7). These are described by the two parallel lines

$$y = \frac{p}{q}x, \quad (9)$$

and

$$y = \frac{p}{q}x + (1 - p) - \frac{p}{q}(1 - q). \quad (10)$$

The available region of the ROC space is thus a parallelogram, the convex hull of the points $(0, 0)$, $(1, 1)$, (q, p) , and $(1 - q, 1 - p)$. An example is depicted in Fig. 1.

In the ROC space, the better a discriminator performs, the closer its representing point is to the point $(0, 1)$ (representing a true positive rate of 1, and a false positive rate of 0). Thus the interesting part of the ROC diagram is the upper piecewise linear curve $(0, 0) \rightarrow \mathbf{P} \rightarrow (1, 1)$, where the point \mathbf{P} is either (q, p) , or $(1 - q, 1 - p)$. In the latter case we can make the substitutions $p \rightarrow 1 - p$ and $q \rightarrow 1 - q$, resulting in the

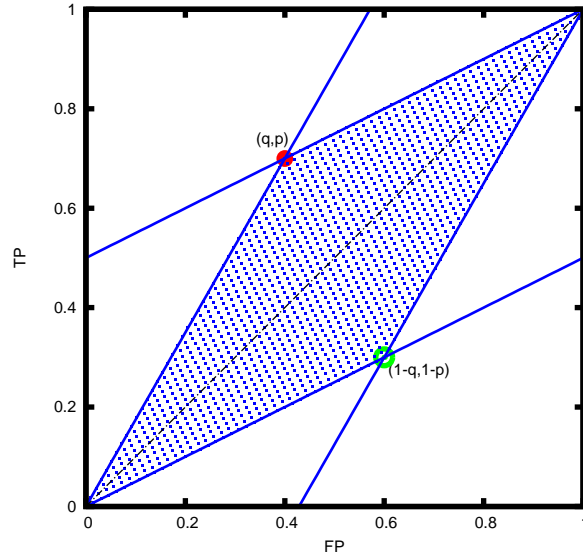


Figure 1. (color online) The available ROC region for the binary variables with $p = 0.7$, $q = 0.4$.

diagram of the same shape, but the two possible \mathbf{P} points interchanged. We may thus always consider $\mathbf{P} = (q, p)$ to be on the upper broken line.

Note that the line representing the best possible discriminators, termed as the “optimal ROC curve” in what follows, connects the points specified by the two possible cumulative distributions $(0, q, 1)$ and $(0, p, q)$ plotted against each other.

It is important to point out that the ROC domain is convex: when considering two points representing two feasible discriminators, all the discriminators whose points are on the line interconnecting the two chosen discriminators on the ROC space are feasible, too. The discriminators on interconnecting line represent discriminators which are defined so that we randomly apply either of the two considered discriminators, according to the evaluation of a random binary variable [3]. Note that the optimal choice of the parameters $p_{a,p}$ and $p_{a,n}$ is not completely trivial. However, at the point (q, p) we have $p_{a,p} = p_{a,n} = 0$, corresponding to the case when we choose to conclude \mathbf{p} if 1 is measured, and \mathbf{n} if 0 is measured, deterministically. Of course, these leads to a TP rate of p and an FP rate of q . The points $(0, 0)$ and $(1, 1)$ correspond to a (though less useful) choice of $p_{a,p} = 0, p_{a,n} = 1$ and $p_{a,p} = 1, p_{a,n} = 0$ respectively. As the available domain is convex, it is indeed plausible that we have the broken line connecting these segments as the ROC curve.

Let us describe the sets of points in the ROC space which correspond to a constant overall probability of failure of the identification, given a prior probability λ . This overall probability reads

$$\begin{aligned} \Pr(\text{fail}) &= \Pr(\mathbf{p}, \mathfrak{N}) + \Pr(\mathbf{n}, \mathfrak{P}) = \Pr(\mathfrak{N}) \Pr(\mathbf{p}|\mathfrak{N}) + \Pr(\mathfrak{P}) \Pr(\mathbf{n}|\mathfrak{P}) \\ &= (1 - \lambda) \Pr(FP) + \lambda(1 - \Pr(TP)). \end{aligned} \quad (11)$$

Thus for a given $\Pr(\text{fail})$, we have a line in the ROC space:

$$\Pr(TP) = \frac{\lambda - \Pr(\text{fail})}{\lambda} + \frac{1 - \lambda}{\lambda} \Pr(FP), \quad (12)$$

with the slope of $(1 - \lambda)/\lambda$.

Finally let us now consider the case of a random variable with N possible values. It can be shown that with the appropriate choice of the mapping of the measurement results (having N possible values in this case) to the conclusion (\mathbf{p} or \mathbf{n}), we get the optimal ROC curve by plotting the two cumulative distributions against each other, and interconnecting the so obtained points with lines, in the descending order of p_i/q_i .

2.2. Bhattacharyya coefficient from the ROC curve

Observe that the shape of the ROC curve is characteristic for the distributions in question: if there are no points with the same p_i/q_i ratio, the curve just determines the two distributions. Only points with the same p_i/q_i introduce a possible ambiguity: they may be interchanged, subdivided into additional points by introducing new possible values of the variables with the same probability ratio, or merged to correspond to the same value.

A prevalently used measure of the similarity of two distributions can be geometrically deduced from the ROC curve. Consider the coordinate transformation

$$\begin{pmatrix} q \\ p \end{pmatrix} \rightarrow \begin{pmatrix} t \\ s \end{pmatrix} = \begin{pmatrix} \frac{p-q}{2} \\ \frac{p+q}{2} \end{pmatrix}, \quad (13)$$

that is, we consider axes rotated by $\pi/4$ counterclockwise to the original ROC axes, and the interchange of their ordering, and shrinking with a factor of $\sqrt{2}$. Further, consider the following Minkowski-metrics defined in terms of the new coordinates:

$$d\ell^2 = ds^2 - dt^2. \quad (14)$$

In the terminology of special relativity the “space” axis will be the original $(0, 0) \rightarrow (1, 1)$ diagonal of the ROC space; while the “time” axis is at right angles to this, pointing upwards. In this way, the part of the domain of the ROC space above the diagonal, where the optimal ROC curve resides, has positive coordinates. Thus the original TP axis is one of the edges of the “future light cone”, while the other axis is that of the “past light cone”. Note that the lines parallel to these axis have zero length in this metric.

Assume that the cumulative distributions

$$P_k = \sum_{l=1}^k p_l \quad (15)$$

and

$$Q_k = \sum_{l=1}^k q_l \quad (16)$$

are plotted against each other, resulting in the ROC curve described in the previous Section. The square of the length ℓ_k of the line segment of the broken line (in Minkowski metric) between the points (Q_k, P_k) and (Q_{k+1}, P_{k+1}) reads

$$\ell_k^2 = - \left(\frac{P_{k+1} - Q_{k+1}}{2} - \frac{P_k - Q_k}{2} \right)^2 + \left(\frac{P_{k+1} + Q_{k+1}}{2} - \frac{P_k + Q_k}{2} \right)^2 \quad (17)$$

$$= - \left(\frac{p_k - q_k}{2} \right)^2 + \left(\frac{p_k + q_k}{2} \right)^2 = p_k q_k. \quad (18)$$

Hence, for the whole length of the broken line in Minkowski metric we have

$$\ell = \sum_k \ell_k = \sum_k \sqrt{p_k q_k} = B(p, q) \quad (19)$$

is the Bhattacharyya-coefficient [4] prevalently used in the literature of statistics. It measures in a way the similarity between two probability distributions.

3. The ROC curves for quantum states

In case of ambiguous quantum state discrimination, we are given a system in an unknown quantum state, but we know in advance that the state is $\varrho_{\mathfrak{P}}$ with probability λ and $\varrho_{\mathfrak{N}}$ with probability $1 - \lambda$. As we discriminate two states, we can assume that we work in a two-dimensional subspace of the Hilbert-space of the studied system, hence, $\varrho_{\mathfrak{P}}$ and $\varrho_{\mathfrak{N}}$ are 2×2 density matrices. They are known a priori, along with $\lambda \in [0, 1]$.

In case of ambiguous state discrimination we have one sample, we are allowed to perform any generalized (POVM) measurement, and we have to decide which one of the two states was given, with the lowest probability of error. The minimum probability of error is given by the well-known Helstrom-formula [7]:

$$P_{E, \min} = \frac{1}{2} (1 - \|\lambda \varrho_{\mathfrak{P}} - (1 - \lambda) \varrho_{\mathfrak{N}}\|_1). \quad (20)$$

In case of ROC analysis, we consider the two possible conclusions \mathfrak{p} (The state was $\varrho_{\mathfrak{P}}$) and \mathfrak{n} (the state was $\varrho_{\mathfrak{N}}$). As for the measurement, we consider the POVM leading to the optimum in the Helstrom formula. This is formed by the spectral projectors associated to the positive and negative eigenvalues of the Hermitian matrix

$$\Lambda = \lambda \varrho_{\mathfrak{P}} - (1 - \lambda) \varrho_{\mathfrak{N}}. \quad (21)$$

3.1. Two pure states

In this Section we consider the discrimination of two pure states. This problem is two-dimensional by nature, so the discrimination of qubit states is the most general as long as mixed states are not considered.

We are given a quantum bit in either of the states

$$|\Psi_{\mathfrak{P}}\rangle = \begin{pmatrix} \cos \frac{\theta_p}{2} \\ \sin \frac{\theta_p}{2} \end{pmatrix} \quad \text{or} \quad |\Psi_{\mathfrak{N}}\rangle = \begin{pmatrix} \cos \frac{\theta_q}{2} \\ \sin \frac{\theta_q}{2} \end{pmatrix} \quad (22)$$

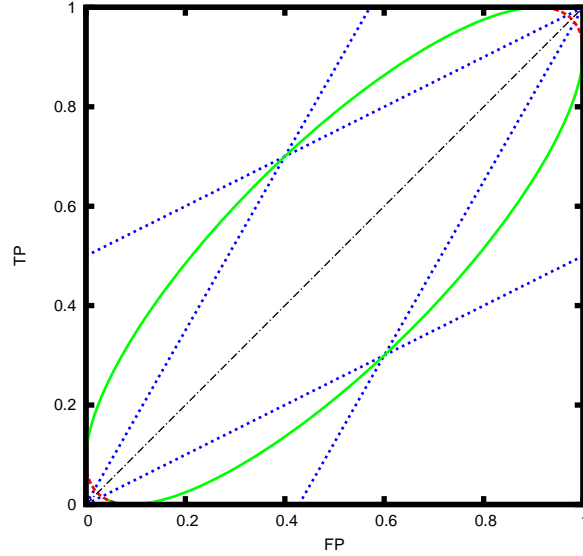


Figure 2. (color online) The ROC curve for two pure quantum states corresponding to the classical binary variables $p = 0.7$, $q = 0.4$ is the ellipse in the figure. For convenience we have also plotted the lines relevant to the classical case. The parts in dashed red are not accessible by using the measurement corresponding to optimal ambiguous discrimination of the states (from the Helstrom formula).

as the “positive” and “negative” case. (To compare with the classical case, set $p = \cos^2(\theta_p/2)$ and $q = \cos^2(\theta_q/2)$ in Eq. (1)). For symmetry reasons we may consider real vectors, but we allow the azimuthal angles θ_p and θ_q to be in the interval $[0, 2\pi[$, thereby obtaining two arbitrary pure states in the $x - z$ plane of the Bloch-sphere.

As the measurement we consider a projective measurement in the basis

$$|\Phi_p\rangle = \begin{pmatrix} \cos \frac{\alpha}{2} \\ \sin \frac{\alpha}{2} \end{pmatrix}, \quad |\Phi_n\rangle = \begin{pmatrix} -\sin \frac{\alpha}{2} \\ \cos \frac{\alpha}{2} \end{pmatrix}, \quad \alpha \in [0, 2\pi[. \quad (23)$$

We assume now that the measurement result corresponding to $|\Phi_p\rangle$ leads to the conclusion that we were given $|\Psi_p\rangle$, and the same holds for the case of “false”. We shall discuss the effect of the classical postprocessing as described in the previous section later.

To obtain the ROC representation we need the false positive and the true positive probabilities, which read, using the same reasoning as in the classical case, after a straightforward calculation,

$$\begin{aligned} \Pr(TP) &= |\langle \Phi_p | \Psi_p \rangle|^2 = \frac{1 + \cos(\alpha - \theta_p)}{2} \\ \Pr(FP) &= |\langle \Phi_n | \Psi_N \rangle|^2 = \frac{1 + \cos(\alpha - \theta_q)}{2}, \end{aligned} \quad (24)$$

again irrespectively of the prior probability of being given either of the possible states. This is apparently the parametric equation of an ellipse. This is visualized in Fig. 2. Our

ellipse's main axis lies on the line $(0, 0) \rightarrow (1, 1)$. The edge points (q, p) and $(1 - q, 1 - p)$ are located on the ellipse. This just means that each of the equations

$$\begin{aligned} \cos\left(\frac{\theta_p}{2}\right)^2 &= \frac{1 + \cos(\alpha - \theta_p)}{2}, \text{ and} \\ \cos\left(\frac{\theta_q}{2}\right)^2 &= \frac{1 + \cos(\alpha - \theta_q)}{2} \end{aligned} \quad (25)$$

indeed do have a solution for α .

Let us now describe the points at which the ellipse touches the edges of the ROC-square. The true positive rate equals to one when $\alpha - \theta_p = 0$, that is, $|\Phi_p\rangle = |\Psi_{\mathfrak{p}}\rangle$. The false positive rate at this point is thus just the fidelity of the two states to be distinguished:

$$\mathcal{F}(\Psi_{\mathfrak{n}}, \Psi_{\mathfrak{p}}) = |\langle \Psi_{\mathfrak{p}} | \Psi_{\mathfrak{n}} \rangle|^2 = |\langle \Phi_p | \Psi_{\mathfrak{n}} \rangle|^2. \quad (26)$$

The false positive rate is one at $\alpha - \theta_q = 0$, thus $|\Phi_p\rangle = |\Psi_N\rangle$, yielding the fidelity again, as

$$\mathcal{F}(\Psi_{\mathfrak{n}}, \Psi_{\mathfrak{p}}) = |\langle \Psi_{\mathfrak{p}} | \Psi_{\mathfrak{n}} \rangle|^2 = |\langle \Psi_{\mathfrak{p}} | \Phi_n \rangle|^2. \quad (27)$$

The true positive rate is zero when $\alpha - \theta_p = \pi$, that is, $\alpha = \pi + \theta_p$ hence $|\Phi_p\rangle = |\Psi_{\mathfrak{p}}^\perp\rangle$, where $|\Psi_{\mathfrak{p}}^\perp\rangle$ is a state orthogonal to $|\Psi_{\mathfrak{p}}\rangle$ in the Hilbert-space. therefore we have for the false positive rate

$$|\langle \Phi_p | \Psi_{\mathfrak{n}} \rangle|^2 = |\langle \Psi_{\mathfrak{p}}^\perp | \Psi_{\mathfrak{n}} \rangle|^2 = 1 - \mathcal{F}(\Psi_{\mathfrak{n}}, \Psi_{\mathfrak{p}}). \quad (28)$$

The point for which the false positive rate is zero is at $\alpha = \theta_n + \pi$, with the true positive rate of $1 - \mathcal{F}(\Psi_{\mathfrak{n}}, \Psi_{\mathfrak{p}})$, which can be justified along the same lines. Hence, we can determine the fidelity of the two states immediately according to the ROC curve.

The classical postprocessing by defining probabilities to accept or reject true or false measurement results in points within the ellipse, making the full area of the ellipse accessible by some setup. Note, that this is ambiguous in the sense that different choices of measurement and postprocessing may result in the same point in the ROC plane.

One may follow a different approach: given the states to be discriminated, and the prior probability λ , we may determine the spectral projectors from Eq. (21), and consider the resulting projective measurements. In this case instead of the direct parameter α of the measurement, we have λ as a parameter. Plotting the resulting points in the ROC curve, we obtain a part of the upper and lower parts of the ellipse, as depicted in Fig. 2. The missing parts of the ellipse (in cyan in the figure) are accessible by the spectral projectors of the overall prior density matrix

$$\rho = \lambda \varrho_{\mathfrak{p}} + (1 - \lambda) \varrho_{\mathfrak{n}}. \quad (29)$$

Thus we have two different interpretations: either given the two states, we may either consider all the possible measurements parametrized by α to obtain the ellipse, or we may consider all the possible prior probabilities λ , and calculate the optimal

measurement, whose corresponding point shall give the upper and lower part of the measurement.

To find the prior probability λ for which a point on the curve in the ROC space is optimal, recall that the curves with a constant overall failure probability are the lines in Eq. (12). Assume that we are in a point at the upper part of the ellipse (i.e. we fix a measurement direction α). Recall also that a point is optimal if it is as close to the point (1,0) as possible. In order to exclude the possibility of decreasing this distance, provided that we fix a prior probability (and thus the slope of the line), the line must be a tangent. The slope of the tangent of the ellipse in the given point is, on the other hand,

$$\frac{\lambda}{1-\lambda} = \frac{d\Pr(TP)}{d\alpha} \left(\frac{d\Pr(FP)}{d\alpha} \right)^{-1} = \frac{\sin(\theta_p - \alpha)}{\sin(\theta_q - \alpha)}. \quad (30)$$

The relation linking the parameter α in our first approach, to the corresponding parameter λ in the second can be found from this equation. In addition, we have an operative notion for the tangents of the ROC curve, which is in fact derives from completely general features of the ROC curve.

It is of some interest to evaluate the classical Bhattacharyya coefficient for the distributions $\Pr(TP), 1 - \Pr(TP)$ and $\Pr(FP), \Pr(1 - FP)$, by substituting these probabilities from Eq. (24) into (19). For the point corresponding to the classical case, it is just the classical coefficient found in Eq. (19). For the upper part of the ellipse, we find that the classical Bhattacharyya coefficient is constant for all the points. Thus the upper ellipse segment corresponding to the different discriminators for two pure qubits (or, otherwise speaking, the optimal discriminators for different prior probabilities λ) are on the isolines of the classical Bhattacharyya coefficient.

3.2. A quantum Bhattacharyya coefficient

According to our experience with the length in Minkowski metric of the upper part of the ROC curve, the question naturally arises whether the same integral for the upper part of the ellipse, from the points where it touches the $0 - 1$ and $1 - 1$ axes is informative for the quantum case. (Note that the optimal ROC curve contains the vertical line connecting the $(FP = 0, TP = 0)$ point to the point of tangency of the ellipse, as well as the horizontal segment from the other point of tangency to the $(FP = 1, TP = 1)$ point, but these are of zero Minkowski-length.

To calculate this we carry out the same transformation as in Eq. (31).

$$\begin{pmatrix} \Pr(FP) \\ \Pr(TP) \end{pmatrix} \rightarrow \begin{pmatrix} t \\ s \end{pmatrix} = \begin{pmatrix} \frac{\Pr(TP) - \Pr(FP)}{\frac{\Pr(TP)^2 + \Pr(FP)}{2}} \\ \frac{\Pr(TP) + \Pr(FP)}{2} \end{pmatrix}, \quad (31)$$

and substitute the results from Eq. (24) into this. We obtain

$$\begin{aligned} t &= \frac{1}{4} ((\cos(\theta_p) - \cos(\theta_q)) \cos(\alpha) + (\sin \theta_p - \sin(\theta_q)) \sin(\alpha)) \\ s &= \frac{1}{4} ((\cos(\theta_p) + \cos(\theta_q)) \cos(\alpha) + (\sin \theta_p + \sin(\theta_q)) \sin(\alpha)). \end{aligned} \quad (32)$$

The length of the curve in Minkowski metric is obtained then as

$$B(|\Psi_{\mathfrak{P}}\rangle, |\Psi_{\mathfrak{N}}\rangle) = \int_{\text{upper curve}} \sqrt{\left(\frac{ds}{d\alpha}\right)^2 - \left(\frac{dt}{d\alpha}\right)^2} d\alpha. \quad (33)$$

As we integrate along the upper part of the curve, we go through alphas from $\Pr(FP) = 0$ to $\Pr(TP) = 1$. In the particular case, however, we have to choose the integration domain to go through the upper curve in the proper direction.

After some algebra we get

$$B(|\Psi_{\mathfrak{P}}\rangle, |\Psi_{\mathfrak{N}}\rangle) = \frac{\sqrt{2}}{4} \int_{\text{upper curve}} \sqrt{\cos(\theta_q + \theta_p) - \cos(\theta_q + \theta_p - 2\alpha)} d\alpha. \quad (34)$$

This leads to elliptic integrals, and can be evaluated numerically. Let us now consider the particular choice of $\theta_p = 0$, and $\theta_q \in [0, \pi]$, thus the positive state points upwards on the Bloch-sphere, while the other one ranging from this state to the one pointing downwards, being orthogonal to the other in the Hilbert-space. This choice covers all the relevant cases. In this case the integral in Eq. (34) reads

$$B(|\Psi_{\mathfrak{P}}\rangle, |\Psi_{\mathfrak{N}}\rangle) = \frac{\sqrt{2}}{4} \int_{\theta_q + \pi}^{2\pi} \sqrt{\cos(\theta_q) - \cos(2\alpha - \theta_q)} d\alpha. \quad (35)$$

This in fact can be expressed in a closed form as

$$B(|\Psi_{\mathfrak{P}}\rangle, |\Psi_{\mathfrak{N}}\rangle) = \frac{1}{4} \left[\frac{2E(x|k) - (1 - \cos \theta)F(x|k)}{\sin\left(\frac{\theta}{2} - \alpha\right)} \right]_{\theta_q + \pi}^{2\pi}, \quad (36)$$

where

$$x = \cos\left(\frac{\theta}{2} - \alpha\right) \sqrt{1 + \cos \theta}, \quad (37)$$

and

$$k = \frac{\sqrt{2}}{2} \sqrt{1 + \cos \theta}, \quad (38)$$

and $F(x|k)$ and $E(x|k)$ are the incomplete elliptic integrals of the first and second kind, respectively.

The dependence of B on θ_q is plotted in Fig. 3. We have plotted the fidelity of the two states, too. We can observe that the fidelity is greater or equal than the Bhattacharyya coefficient (equal for the values 0 and 1). Both are monotonously decreasing.

3.3. Two qubits

Now we generalize our ideas to the general two-dimensional case, that is, we allow the two states to be mixed, described by the two-dimensional density operators $\varrho_{\mathfrak{P}}$ and $\varrho_{\mathfrak{N}}$.

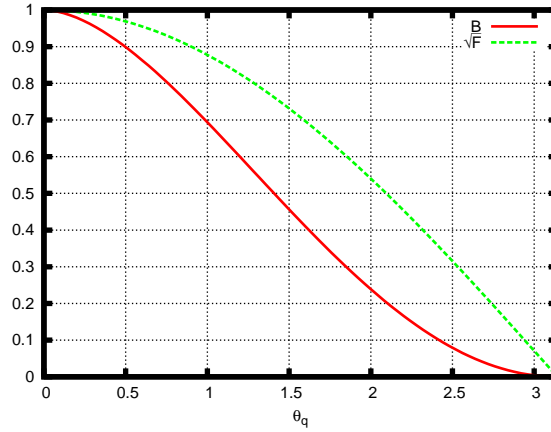


Figure 3. (color online) The quantum Bhattacharyya coefficient in Eq. (33), and the square root fidelity of the two states for $\theta_p = 0$, as a function of θ_q .

On the Bloch-sphere, each of them can be written as $\varrho = 1/2(\hat{1} + \mathbf{r}\sigma)$, where \mathbf{r} is the real 3-vector representing the state, while σ contains the three Pauli matrices. For pure states, the \mathbf{r} -s are unit vectors. The coordinates of the ROC curve in general read

$$\begin{aligned} \Pr(TP) &= \text{tr}(M_p \varrho_{\mathfrak{P}}) \\ \Pr(FP) &= \text{tr}(M_p \varrho_{\mathfrak{N}}), \end{aligned} \quad (39)$$

where M_p is the measurement operator for the positive conclusion. As trace is linear, and thus these expressions are inhomogeneous linear functions of the Bloch-vectors \mathbf{r}_P and \mathbf{r}_N , the ellipse we found in the case of two pure states is just shrunk anisotropically to the point $(1/2, 1/2)$. (The TP and FP directions shrink proportionally with the length of the respective Bloch-vectors.) For mixed states, this does not touch the edges of the ROC space anymore. However, as the $(0, 0) \rightarrow (1, 1)$ line is necessarily part of the feasible ROC domain, the upper part of the ROC curve we are looking for is the convex hull of the (shrunk) ellipse and the points $(0, 0)$, $(1 - 1)$.

Recall that the ellipses found in 3.1 for two pure states are the iso-Bhattacharyya lines, and they touch the edges of the ROC space at points described by the fidelity of the two states. In case of mixed states, the square root fidelity is the minimum of the classical square root fidelities, that is, the Bhattacharyya coefficients of the classical probability distributions the two quantum states can yield when measured [5, 8]. Hence, to find the square root quantum fidelity we need to find the iso-Bhattacharyya ellipse which is tangent to the shrunk ellipse. The tangent point will give the optimal discriminator. The square root fidelity of the two mixed states is determined by the points where the tangent iso-Bhattacharyya ellipse touches the edges of the ROC space. Note that this consideration is valid for two dimensional states (that is, the two density operators' common support is two dimensional). For higher dimensional classical distributions there are no iso-Bhattacharyya curves, the existence of which is due to the fact that a pair of distributions is characterized by a single point in the ROC space.

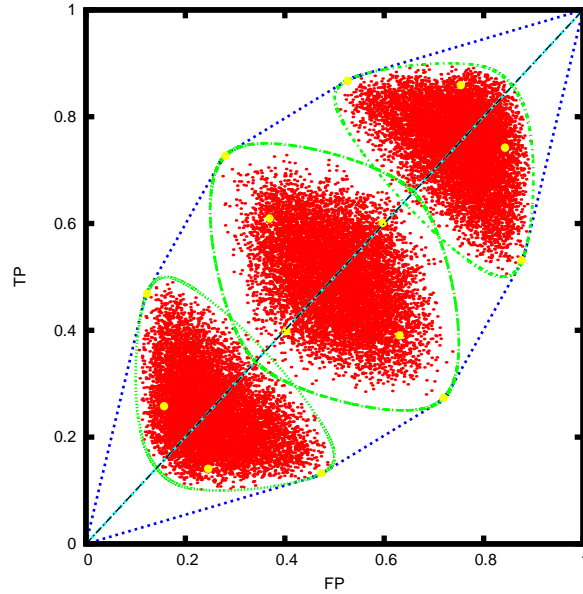


Figure 4. (color online) ROC curve/space of to randomly selected 4 dimensional density matrices. The dash-dotted (green) closed curves are regions accessible with rank 1, 2 and 3 projectors, respectively. The dotted (blue) curve is the actual ROC curve, according to the Helstrom formula. The scattered small (red) dots are randomly (according to the Haar measure) selected projectors. The bigger, lighter (yellow) points are the those corresponding to the optimal fidelity measuring observables defined by Eq. (44).

3.4. Two arbitrary quantum states

Let us now omit any restriction, and consider $\varrho_{\mathfrak{P}}$ and $\varrho_{\mathfrak{N}}$ in an arbitrary Hilbert-space. In this case we also need to obtain a convex domain in the ROC space, whose upper edge is a ROC curve corresponding to potentially optimal discrimination.

This upper edge can be obtained by calculating the convex hull of the points corresponding to different projective measurements resulting from the Helstrom formula, for all possible prior probabilities λ . The projective measurements $M_{\mathfrak{p}}, M_{\mathfrak{n}}$ resulting from the Helstrom formula are projectors onto the positive vs. negative spectral subspace of the matrix Λ in Eq. (21). Hence, the parts of the curve resulting from the Helstrom formula directly have discontinuities: when the rank of $M_{\mathfrak{p}}$ changes (due to the change of sign of an eigenvalue of Λ), there is a split.

Alternatively we may just pick the two states and calculate all the probabilities for all possible pairs of orthogonal projectors. If the density operators' common support is n dimensional, the examined projectors' rank should range from 0 to n . Each rank will result in a convex spot around the line $(0,0), (1,1)$ in the ROC space (for dimensions 0 and n , we get the points $(0,0)$ and $(1,1)$ respectively). The convex hull of these will describe the accessible domain in the ROC space, and its upper part will be our ROC curve. This is illustrated in Fig. 4.

Note that as the constant failure probability curves are the lines in Eq. (12) (this

is a general property of the ROC space), the tangents of the ROC curve have the same operational meaning as in the case of pure states: the tangent points give the optimal discriminator for the given prior.

3.4.1. Trace distance The ROC curve also yields a geometric notion of the trace distance. Assume that we have equal prior probabilities, i.e., $\lambda = 1/2$. Recall that according to Eq. (30), the optimal discriminator at the ROC curve is its point of tangency with its 45 degree tangent, i.e. the one parallel to the $(0,0) - (1,1)$ line. On the other hand, this discriminator is obtained from the Helstrom formula, as the projective measurement M_p, M_n onto the positive vs. negative spectral subspace of the matrix Λ in Eq. (21), which in the present case reads

$$\Lambda = \frac{1}{2}(\varrho_{\mathfrak{P}} - \varrho_{\mathfrak{N}}). \quad (40)$$

The trace distance is defined as [5]

$$d_{\text{tr}}(\varrho_{\mathfrak{P}}, \varrho_{\mathfrak{N}}) = \frac{1}{2} \text{tr} |\varrho_{\mathfrak{P}} - \varrho_{\mathfrak{N}}| = \text{tr} |\Lambda|. \quad (41)$$

(Note that we use the definition having the factor $1/2$ included.) It can be written as

$$2d_{\text{tr}}(\varrho_{\mathfrak{P}}, \varrho_{\mathfrak{N}}) = \text{tr}(M_p(\varrho_{\mathfrak{P}} - \varrho_{\mathfrak{N}})) + \text{tr}(M_n(\varrho_{\mathfrak{P}} - \varrho_{\mathfrak{N}})). \quad (42)$$

As Λ is traceless, the two summands on the right hand side are equal, thus we have

$$d_{\text{tr}}(\varrho_{\mathfrak{P}}, \varrho_{\mathfrak{N}}) = \text{tr}(M_p(\varrho_{\mathfrak{P}} - \varrho_{\mathfrak{N}})) = \text{Pr}(TP) - \text{Pr}(FP). \quad (43)$$

This is just the intersection of the 45 degree tangent with the TP axis. The trace distance can be thus read directly from the ROC curve.

3.5. The quantum Bhattacharyya coefficient

Following the line of thought of the previous sections, we finally analyze the possibility of introducing a quantum Bhattacharyya coefficient as we did for two pure states in Section 3.2. Apart from the particular shape of the ROC curve, we have not exploited any property stemming from the quantum scenario. Hence, we may call the length of the ROC curve in Minkowski metric a quantum Bhattacharyya coefficient. This can be considered as a novel quantity to measure the similarity of the states. It can be evaluated numerically, in a straightforward but somewhat laborious way. We consider here its general properties here instead.

Proposition 1. *The quantum Bhattacharyya coefficient is zero if and only if the two states can be distinguished with certainty (i.e., the two density operators have disjoint support), and one if and only if the two states are the same.*

Proof. In the first case, the ROC curve is the $(0 - 0) \rightarrow (0,1) \rightarrow (1,1)$ broken line, which is the only one with zero length in this metric, while in the latter case it is the $(0,0) \rightarrow (1,1)$ line, which is the longest line in the ROC space in this metric. \square

Lemma 1. *Given two convex curves, the outer one (that is, which runs above the other in the ROC space) is shorter in the Minkowski metrics.*

Proof. Consider the midpoint of the inner (lower) curve, and draw a tangent to it. This tangent intersects the outer (upper) curve at two points. Let us replace the outer curve by the line segment between these two points. Thereby we have increased its length in the Minkowski metric. (If the two points are on both of the original curves, we skip this step.) Let us repeat this procedure with the points at 1/4 and 3/4 of the outer curve. By the replacements we increase the length of the outer curve. Upon repeating the procedure we get an arbitrarily fine approximation of the inner curve, and their Minkowski length shall be equal. As during the procedure we have not decreased the Minkowski length, the outer curve should have been shorter than the inner one. (Note that we have not even exploited the fact that the outer curve was convex.) \square

Proposition 2. *The quantum Bhattacharyya coefficient is lower than or equal to the square root fidelity. It is equal if and only if the two density operators commute.*

Proof. It is known that there exists an optimal projective measurement, for which the Bhattacharyya coefficient of the classical measurement result is the square root of the fidelity. (In particular, the observable is

$$M = \frac{1}{\sqrt{\varrho_{\mathfrak{N}}}} \sqrt{\sqrt{\varrho_{\mathfrak{N}}} \varrho_{\mathfrak{P}} \sqrt{\varrho_{\mathfrak{N}}}} \frac{1}{\sqrt{\varrho_{\mathfrak{N}}}}, \quad (44)$$

c.f Eq. (13.54) of Ref. [5]. This obviously defines $d+1$ points in the feasible ROC domain, where d stands for the dimension of the joint support of the two density operators. (It is an interesting open question whether these points are actually on the optimal ROC curve.) These points define a sequence of line segments in the feasible ROC domain, starting from $(0,0)$, ending at $(1,1)$. It is obviously convex, and goes below the real ROC curve. If the two density operator commute, then the ROC curve coincides with this polyline, as the measurement itself becomes classical. Otherwise the convex curve necessarily goes above its chords. The statement then follows from Lemma 1. \square

Proposition 3. *The quantum Bhattacharyya coefficient is monotone under completely positive maps.*

Proof. In order to see this we need to consider the whole domain in the ROC space which is accessible via a POVM in the ROC space (whose upper border is the ROC curve). Importantly this is symmetric to the point $(1/2, 1/2)$: for an arbitrary point in the domain, the classical negation of the measurement result yields its reflected counterpart. In the Heisenberg picture, a completely positive (CP) map transforms a POVM into another POVM. Hence, such a transformation cannot lead out of the original accessible domain, but some points may become inaccessible. Thus the domain will shrink (or remain the same), and it will be of course still convex, as it is the ROC region of the new states. Thus the transformed ROC curve will be the same or below the upper curve, which has a higher length in the Minkowski metric according to Lemma 1 \square

We remark here that the parts of the ROC domain belonging to a given rank of the projectors themselves are not contracted as described above, in general. We conjecture that for unital maps, however, they will be contracted, too.

4. Unambiguous quantum state discrimination

Using the ROC technique we have introduced thus far can be fruitful in the understanding of unambiguous quantum state discrimination, too. Consider two arbitrary quantum states, the “positive” and “negative” one. (They do not need to be pure, neither of common support.) We are looking for a POVM of 3 operators: M_p detecting the positive state with certainty, M_n the negative one with certainty, and the third one, $M_? = \hat{1} - M_p - M_n$ resulting in the inconclusive outcome.

The first idea is to consider to merge one of the conclusive outcomes with the inconclusive one. If the negative one is merged, this results in an ambiguous discrimination problem, with a TP rate of one, however. So it has a point in the ROC space, and it should be on the line $(0, 1) \rightarrow (1, 1)$. If the positive one is merged, the negative state is identified with certainty, thus we are on the TP axis. This confirms very transparently the otherwise known fact that it is a necessary condition for the availability of an unambiguous discrimination that the ROC domain of the states touches both the TP axis and the line $(0, 1) \rightarrow (1, 1)$. (Excluding the trivial points $(0, 0)$ and $(1, 1)$ of course.)

Next we show that it is a sufficient condition as well. Consider a pair of states which satisfy this condition. For each of the points mentoned in the condition, we have a projective measurement, with the property that one of its elements identifies one of the states with certainty, as they project onto the other density operator’s null space. The Helstrom-formula provides us with these projectors. (In fact, we may also use a positive measurement operator that maps into the respective null-space.) Let us denote these projectors by \tilde{M}_p and \tilde{M}_n . These projectors can be derived from the Helstrom formula, too. Note that they need not be rank one projectors in general. Their rank is between 1 and $d - 1$, d standing for the dimension of the common support of the states, for if any of them has full rank, the respective measurement will not yield any information. Hence, if the two density operators have fully overlapping supports, the states cannot be unambiguously discriminated.

If we do have nontrivial \tilde{M}_p and \tilde{M}_n , there exist $\lambda_1, \lambda_2 \in]0, 1]$ so that $\lambda_1 \tilde{M}_p + \lambda_2 \tilde{M}_n \leq \hat{1}$. E.g. $\lambda_1 = \lambda_2 = 1/2$ is a suitable choice. The choice of the λ -s can tune the success probability of the detection in favor one of the states and to the detriment of the other. Choosing $\tilde{M}_? = \hat{1} - \tilde{M}_p - \tilde{M}_n$ completes the two operators the triplet $\tilde{M}_p, \tilde{M}_n, \tilde{M}_?$ which is a POVM that implements the unambiguous discrimination, not necessarily optimally though.

5. Conclusions

We have presented the ROC analysis of the task of distinguishing two quantum states, providing an intuitive representation of the problem. The trace distance of two arbitrary states, and the fidelity of a pair of states with a two-dimensional common support can be directly read out from the ROC diagram. We have also discussed to some extent the case of unambiguous discrimination in this picture.

We have introduced a quantum generalization of the classical Bhattacharyya coefficient as the length in Minkowski metric of the optimal ROC curve for two arbitrary states. While it is a natural generalization of the classical Bhattacharyya coefficient as evaluated using the ROC curve, it has a notion which is different from the earlier definitions of the quantum Bhattacharyya coefficient. We have shown that this quantity is a lower bound for the fidelity, with equality if and only if the states commute. As it is zero for distinguishable states whereas it is one if the two states are the same, it can be used to measure indistinguishability of quantum states. In addition, it is monotone under completely positive maps.

Even though the facts covered by our present analysis are not novel, they appear here in a comprehensive picture which supports a useful way of thinking about the problem. We believe that this deepens the understanding of the nature of the problem of distinguishing quantum states. In addition, the present approach may prove to be useful in understanding other strategies of quantum state discrimination as well as more complex topics such as the discrimination of quantum channels, etc.

The alternative quantum Bhattacharyya coefficient which we have introduced is a natural generalization of the classical one, and even though it is not straightforward to calculate it for particular states, its notion and behavior is very transparent from the knowledge of the ROC curve. In addition, we found that it has properties which are commonly expected from a well-behaved quantum distinguishability measure.

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